5s correlation confinement resonances in Xe-endo-fullerenes

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Synopsis Spectacular trends in the modification of the Xe 5s photoionization via interchannel coupling with confinement resonances emerging in the Xe 4d giant resonance upon photoionization of the Xe@C_{60}, Xe@C_{240} and Xe@C_{60}@C_{240} endo-fullerenes are theoretically unraveled and interpreted.

Resonances, termed *confinement resonances* (CR's), emerging in photoionization spectra of atoms A confined inside the empty spaces of endo-fullerenes - A@C_n, A@C_n@C_m, *etc* - have attracted much attention of investigators in recent years [1] (and references therein). CR's occur in endo-fullerene photoionization spectra due to the interference of the photoelectron waves emerging directly from the confined atom A, and those scattered off the endo-fullerene confining cage(s). Their existence has recently been confirmed experimentally [2]. *Correlation confinement resonances* (CCR's) differ from ordinary CR's in that they occur in the photoionization of an *outer* subshell of the confined atom A due to the interference of transitions from the outer subshell with ordinary CR's emerging in *inner* shell photoionization transitions, via interchannel coupling [1, 3]. They were originally theoretically discovered in the Xe 5s photoionization of Xe@C_{60} [3]. The CCR phenomenon thus introduces a novel class of resonances that can exist neither without a confinement nor electron correlation, thereby attracting much interest to their study.

Ordinary CR's in the Xe 4d giant photoionization resonance undergo dramatic changes along the path from Xe@C_{60} to Xe@C_{240} to Xe@C_{60}@C_{240} [4]. With the impetus of results of Ref. [4], we study how ordinary CR's in the Xe 4d photoionization affect the Xe 5s photoionoization in various Xe-endo-fullerenes. It is the aim of this paper to report on spectacular CCR's emerging in the Xe 5s photoionization cross section due to interchannel coupling of the 5s $\to$ p transition with transitions from the Xe inner 4d subshell, and how these CCR's change along the path Xe@C_{60} $\to$ Xe@C_{240} $\to$ Xe@C_{60}@C_{240}.

In performed calculations, fullerene cages were approximated by square-well potentials of certain inner radii r_0, widths Δ and depths U_0 [1, 3]. The Xe atom was placed at the center of fullerenes, both single-cage and nested fullerenes. The updated values of $\Delta \approx 1.25$, $r_0 \approx 6.01$ and $U_0 \approx -0.422$ *au* [4] for C_{60} were used in calculations. This is because they were shown [4] to provide a closer agreement between experiment theory. As for C_{240}, $\Delta \approx 1.25$, $r_0 \approx 12.875$ and $U_0 \approx -0.52$ *au* [4]. Interchannel coupling was accounted for in the framework of the random phase approximation with exchange [5]. The calculated data are depicted in figure 1 where spectacular changes in the Xe 5s photoionization along the path Xe@C_{60} $\to$ Xe@C_{240} $\to$ Xe@C_{60}@C_{240} are seen. A detailed discussion will be offered at the spot.

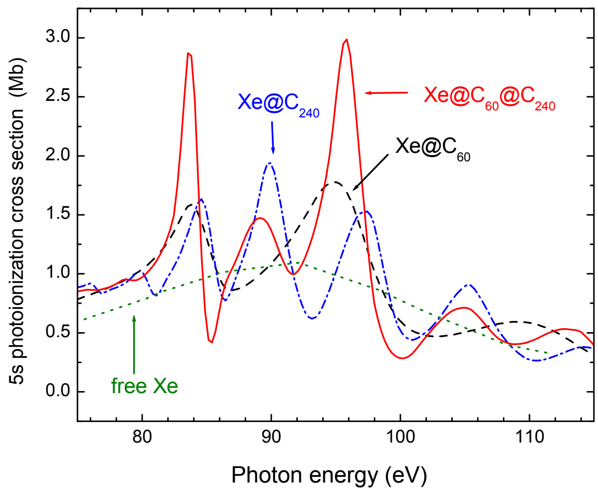

Figure 1. Correlation confinement resonances in the Xe 5s photoionization cross section of Xe@C_{60}, Xe@C_{240} and Xe@C_{60}@C_{240}, as marked. They "mirror" CR's in the Xe 4d photoionization cross sections (not shown) of the endo-fullerenes in questions [4], due to interchannel coupling.

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References

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